UNIVERSITI SAINS MALAYSIA

First Semester Examination
2012/2013 Academic Session

January 2013

EKC 336 – Chemical Reaction Engineering
[Kejuruteraan Tindak Balas Kimia]

Duration : 3 hours
[Masa : 3 jam]

Please check that this examination paper consists of SIX pages of printed material and SIX pages of Appendix before you begin the examination.

[Sila pastikan bahawa kertas peperiksaan ini mengandungi ENAM muka surat yang bercetak dan ENAM muka surat Lampiran sebelum anda memulakan peperiksaan ini.]

Instruction: Answer **ALL** (4) questions.

*[**Arahan:** Jawab **SEMUA** (4) soalan.]*

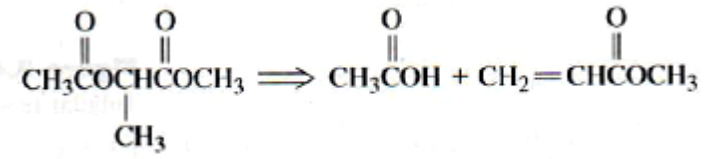
In the event of any discrepancies, the English version shall be used.

[Sekiranya terdapat sebarang percanggahan pada soalan peperiksaan, versi Bahasa Inggeris hendaklah diguna pakai.]

Answer ALL questions.
Jawab SEMUA soalan.

1. [a] A Plug Flow Reactor (PFR) operating isothermally at 773 K is used to conduct the following reaction:

Sebuah reaktor palam aliran beroperasi secara isoterma pada 773K digunakan untuk menjalankan tindak balas berikut:



methylacetoxypropionate	acetic acid	methyl acrylate
metilasitoksipropionat	*asid asetik*	*metil akrilat*

If a feed of pure is the methylacetoxypropionate enters at 5 atm and at a flow rate of 20 m^3/h, what the length of pipe with a cross-sectional area of 0.0036 m^2 is necessary for the reaction to achieve 90 percent conversion?

Jika suapan tulen metilasitoksipropionat masuk pada 5 atm dan kadar aliran 20 m^3/j, apakah panjang paip yang mempunyai luas keratan rentas 0.0036 m^2 yang diperlukan bagi tindak balas untuk mencapai penukaran 90 peratus?

Data: $k = 7.8 \times 10^9 \exp[-19{,}200/T], (s^{-1})$

[10 marks/markah]

[b] The trimerization
Trimerizasi ini

$$3A(g) \rightarrow A_3(g,l)$$

is carried out isothermally and without pressure drop in a PFR at 298 K and 2 atm. As the concentration of A_3 increases downstream the reactor and A_3 begins to condense. The vapor pressure of A_3 at 298 K is 0.5 atm. If an equal molar mixture of A and inert, (I) is fed into the reactor, at what conversion of A will A_3 begin to condense?

dijalankan secara isoterma dan tanpa kejatuhan tekanan di dalam sebuah reaktor palam aliran pada 298K dan 2 atm. Kepekatan A_3 meningkat dihilir reaktor dan A_3 mula untuk terpeluwap. Tekanan wap A_3 pada 298K adalah 0.5 atm. Jika campuran molar sama bagi A dan lengai, (I) disuapkan ke dalam reaktor, pada penukaran berapakah A akan bermula memeluwapkan A_3?

[8 marks/markah]

[c] Starting from general mole balance equation, derive the design equation for PFR.

Bermula dari persamaan umum keseimbangan mol, terbitkan persamaan rekabentuk untuk reaktor palam aliran.

[7 marks/markah]

2. [a] The decomposition of a halogen was studied, with the results shown in Table Q.2.[a].:

Penguraian halogen tleah dipelajari, dengan keputusan yang ditunjukkan di dalam Jadual S.2.[a].:

$$A_2 \xrightarrow{UV} products$$

$$A_2 \xrightarrow{UV} produk$$

Table Q.2.[a].
Jadual S.2.[a].

Time (Min) ***Masa (Min)***	**C_A (ppm)**
10	2.45
20	1.74
30	1.23
40	0.88
50	0.62
60	0.44

Use the differential method of analysis to determine the rate law, then calculate the required rate of addition (in units of lb/hr) of this halogen necessary to maintain a concentration of 1 ppm in a sun-illuminated, 25,000 gallon pond.

Gunakan analisis kaedah pembezaan untuk menentukan hukum kadar, kemudian kirakan kadar yang diperlukan untuk penambahan (dalam unit lb/j) bagi keperluan halogen untuk mengekalkan kepekatan 1 ppm di bawah pencahayaan matahari bagi 25,000 gelen kolam.

(Note: ppm parts of bromine per million parts brominated water by weight. In dilute aqueous solutions, 1 ppm=1 milligram per liter, molecular weight of Br = 80 Daltons.)
(Nota: bahagian ppm bagi bromin per bahagian juta dibrominkan dengan air berdasarkan berat. Bagi larutan akuas tercair, 1 ppm = 1 miligram per liter, berat molekul Br = 80 Dalton).

1 gal $\longrightarrow$ 3.785 liter
1 lb $\longrightarrow$ 454 g

[15 marks/markah]

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[b] [i] Prepare a stoichiometric table showing the effluent concentrations of all species of a gas-phase PFR for the stoichiometry $A \rightarrow B + 2C$. The reactor feed contains half (molar) inert.

Sediakan jadual stoikiometri yang menunjukkan kepekatan keluar bagi semua spesis fasa gas reaktor palam aliran untuk stoikiometri $A \rightarrow B + 2C$. Suapan reaktor mengandungi separuh (molar) lengai.

[ii] Using the results in the stoichiometric table prepared in Q.2.[b].[i]., define an elementary rate law in terms of conversion.

Gunakan keputusan di dalam jadual stoikiometri yang disediakan dalam S.2.[b].[i]., takrifkan hukum kadar asas berdasarkan penukaran.

[iii] By what fraction does C_A change at 80% conversion?
Berapakah pecahan bagi C_A bertukar kepada 80% penukaran?

[10 marks/markah]

3. [a] The complex reactions
Tindak balas kompleks

$$A \xrightarrow{k1} B$$
$$B \xrightarrow{k2} C$$
$$B \xrightarrow{k3} D$$

were carried out with pure A as feed.
telah dijalankan dengan A tulen sebagai suapan.

[i] Derive an equation for A concentration as a function of time in a batch reactor. If $k_1 = 0.01\ s^{-1}$, what is the ratio of C_A/C_{A0} after 1.5 min?

Terbitkan persamaan untuk kepekatan A sebagai fungsi masa dalam reaktor berkelompok. Jika $k_1 = 0.01\ s^{-1}$, apakah nisbah C_A/C_{A0} selepas 1.5 min?

[5 marks/markah]

[ii] If the series reaction is carried out in a continuos stirred reactor (CSTR), determine the reactor volume that will maximize the production of B for a volumetric flow rate of 20 dm^3/min. Please note that $k_2 = 0.003\ s^{-1}$, $k_3 = 0.002\ s^{-1}$ and $C_{A0} = 0.2$ g mol/dm^3. (Hint: $dC_B/dt = 0$)

Jika tindak balas bersiri ini dijalankan di dalam reaktor pengaduk berterusan, tentukan isipadu reaktor yang akan memaksimumkan pengeluaran B untuk kadar aliran isipadu sebanyak 20 dm^3/min. Sila ambil perhatian bahawa $k_2 = 0.003\ s^{-1}$, $k_3 = 0.002\ s^{-1}$ dan $C_{A0} = 0.2$ g mol/dm^3. (Petunjuk: $dC_B / dt = 0$)

[10 marks/markah]

[b] The decomposition of ozone can be accelerated in the presence of a catalyst such as chlorine atoms or radicals in the presence of fluorochlorocarbons.

Penguraian ozon boleh dipercepatkan dalam kehadiran pemangkin seperti atom klorin atau radikal dalam kehadiran fluoroklorokarbon.

$$O + O_3 \xrightarrow{Cl} 2O_2$$

The decomposition mechanisms are stated as below.

Mekanisma penguraian dinyatakan seperti di bawah.

$$CF_2Cl_2 \xrightarrow[<220_{nm}]{h\nu} Cl + CF_2Cl$$

$$Cl + O_3 \xrightarrow{k1} O_2 + ClO$$

$$ClO + O \xrightarrow{k2} Cl + O_2$$

Demonstrate that the decomposition rate is in the form of
Tunjukkan bahawa kadar penguraian adalah dalam bentuk

$$-r_{O3} = k_2 C_{cl}^{\ T} C_O$$

where $C_{Cl}^{\ T} = C_{Cl} + C_{ClO}$ is constant

di mana $C_{Cl}^{\ T} = C_{Cl} + C_{ClO}$ *adalah malar.*

[10 marks/markah]

4. [a] An elementary and irreversible reaction (A → R) occurs in a CSTR. The following information is given.

Satu tindak balas asas dan tidak berbalik (A → R) berlaku di dalam reaktor pengaduk berterusan. Maklumat yang berikut diberikan.

$$-r_A = e^{25} e^{-20000/RT} C_A \, (mol/L.min)$$

$$C_{A0} = 1 mol/L$$

$$T_0 = 350K$$

$$\Delta H_{RA} = -100{,}000 (cal/molA)$$

$$\rho C_P = 500 (cal/L.°C)$$

[i] Determine the reactor space time (τ) and heat to be removed for achieving 90 % of conversion at 350 K.

Tentukan masa ruang reaktor (τ) dan haba yang perlu dibebaskan untuk mencapai 90% penukaran pada 350 K.

[4 marks/markah]

[ii] Determine the maximum adiabatic temperature and reactor space time (τ) needed for achieving 90% of conversion if the reaction is conducted adiabatically.

Tentukan suhu maksimum adiabatik dan reaktor masa ruang (τ) yang diperlukan untuk mencapai 90% penukaran jika tindak balas dijalankan secara adiabatik.

[6 marks/markah]

[b] [i] Determine mean residence time ($\bar{t}$) and plot the residence time distribution (E(t)) from a cumulative distribution curve of a step response in Figure Q.4.[b].

Tentukan purata masa mastautin ($\bar{t}$) dan plotkan taburan masa mastautin (E(t)) daripada lengkung taburan kumulatif bagi satu sambutan langkah dalam Rajah S.4.[b].

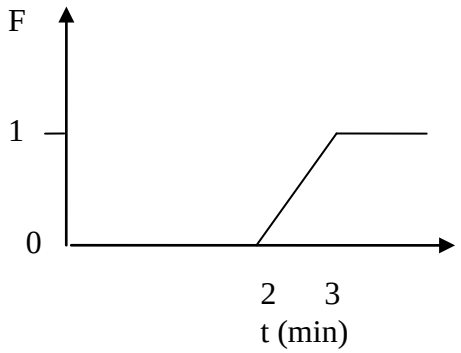

Figure Q.4.[b].
Rajah S.4.[b].

[5 marks/markah]

[ii] An impulse tracer test produced the exit age distribution function presented in Table Q.4.[b]., for a reactor with a first-order reaction (rate constant k = 0.1 min^{-1}). Find the reactant conversion for two different assumptions which are ideal plug flow and perfect mixing. What do you expect on the real conversion?

Satu ujian pengesan dedenyut menghasilkan fungsi taburan umur keluar yang dibentangkan dalam Jadual S.4.[b]., untuk satu reaktor dengan tindak balas tertib pertama (pemalar kadar k = 0.1 min^{-1}). Carikan penukaran bahan tindak balas untuk dua andaian yang berbeza, iaitu aliran palam yang ideal dan percampuran sempurna. Apa yang anda ramalkan pada penukaran sebenar?

Table Q.4.[b].
Jadual S.4.[b].

t (min)	0	5	10	15	20	25	30	35	40
E(t) (min^{-1})	0	0.030	0.050	0.050	0.040	0.020	0.010	0.002	0

[10 marks/markah]

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Appendix

Numerical Techniques A

A.1 Useful Integrals in Reactor Design

Also see http://www.integrals.com

$$\int_0^x \frac{dx}{1-x} = \ln\frac{1}{1-x} \tag{A-1}$$

$$\int_0^x \frac{dx}{(1-x)^2} = \frac{x}{1-x} \tag{A-2}$$

$$\int_0^x \frac{dx}{1+\varepsilon x} = \frac{1}{\varepsilon}\ln(1+\varepsilon x) \tag{A-3}$$

$$\int_0^x \frac{1+\varepsilon x}{1-x}\,dx = (1+\varepsilon)\ln\frac{1}{1-x} - \varepsilon x \tag{A-4}$$

$$\int_0^x \frac{1+\varepsilon x}{(1-x)^2}\,dx = \frac{(1-\varepsilon)x}{1-x} - \varepsilon\ln\frac{1}{1-x} \tag{A-5}$$

$$\int_0^x \frac{(1+\varepsilon x)^2}{(1-x)^2}\,dx = 2\varepsilon(1+\varepsilon)\ln(1-x) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 x}{1-x} \tag{A-6}$$

$$\int_0^x \frac{dx}{(1-x)(\Theta_B - x)} = \frac{1}{\Theta_B - 1}\ln\frac{\Theta_B - x}{\Theta_B(1-x)} \qquad \Theta_B \neq 1 \tag{A-7}$$

$$\int_0^x \frac{dx}{ax^2+bx+c} = \frac{-2}{2ax+b} + \frac{2}{b} \qquad \text{for } b^2 = 4ac \tag{A-8}$$

$$\int_0^x \frac{dx}{ax^2+bx+c} = \frac{1}{a(p-q)}\ln\left(\frac{q}{p}\cdot\frac{x-p}{x-q}\right) \qquad \text{for } b^2 > 4ac \tag{A-9}$$

$$\int_0^W (1-\alpha W)^{1/2}\,dW = \frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right] \tag{A-10}$$

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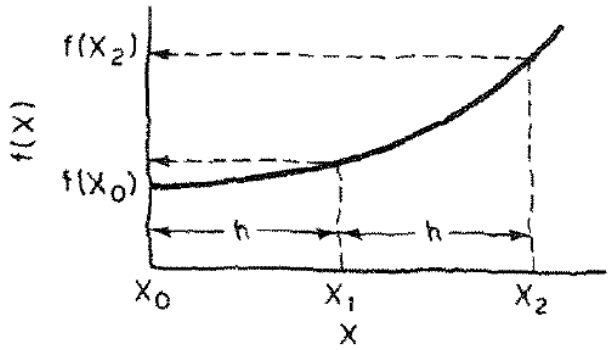
Simpson's one-third rule (three-point) (Figure A-3). A more accurate evaluation of the integral can be found with the application of Simpson's rule:

$$\int_{X_0}^{X_2} f(X)\,dX = \frac{h}{3}[f(X_0) + 4f(X_1) + f(X_2)] \qquad \text{(A-20)}$$

where

$$h = \frac{X_2 - X_0}{2} \qquad X_1 = X_0 + h$$



oix **Figure A-3** Simpson's three-point rule illustration. 11

Simpson's three-eighths rule (four-point) (Figure A-4). An improved version of Simpson's one-third rule can be made by applying *Simpson's second rule*:

$$\int_{X_0}^{X_3} f(X)\,dX = \tfrac{3}{8}h[f(X_0) + 3f(X_1) + 3f(X_2) + f(X_3)] \qquad \text{(A-21)}$$

where

$$h = \frac{X_3 - X_0}{3} \qquad X_1 = X_0 + h \qquad X_2 = X_0 + 2h$$

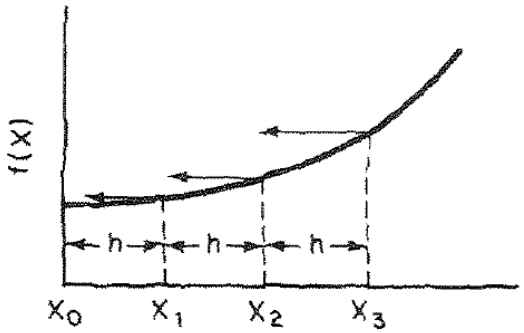


Figure A-4 Simpson's four-point rule illustration.

Ideal Gas Constant

$$R = \frac{8.314\ \text{kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}} \qquad R = \frac{1.987\ \text{Btu}}{\text{lb mol} \cdot {}^\circ\text{R}}$$

$$R = \frac{0.73\ \text{ft}^3 \cdot \text{atm}}{\text{lb mol} \cdot {}^\circ\text{R}} \qquad R = \frac{8.3144\ \text{J}}{\text{mol} \cdot \text{K}}$$

$$R = 0.082\ \frac{\text{dm}^3 \cdot \text{atm}}{\text{mol} \cdot \text{K}} = \frac{0.082\ \text{m}^3 \cdot \text{atm}}{\text{kmol} \cdot \text{K}} \qquad R = \frac{1.987\text{cal}}{\text{mol} \cdot \text{K}}$$

Temperature

°F = 1.8 × °C + 32
R = °F + 459.69
K = °C + 273.16
°R = 1.8 × K
°Réamur = 1.25 × °C

First Point $$\left.\frac{dC_A}{dt}\right|_{t_0} = \frac{-3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t}$$

Interior Points or Median $$\left.\frac{dC_A}{dt}\right|_{t_i} = \frac{C_{A\,(i+1)} - C_{A(i-1)}}{2\Delta t}$$

Last Point or Third quartile $$\left.\frac{dC_A}{dt}\right|_{t_n} = \frac{C_{A(n-2)} - 4C_{A\,(n-1)} + 3C_{A(n)}}{2\Delta t}$$

Useful differential equations:

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}$$

$$\frac{d}{dx}(u/v) = \frac{(v\frac{du}{dx} - u\frac{dv}{dx})}{v^2}$$

…4/-

Numerical Evaluation of Integrals:

1. Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] \text{ when } h = x_1 - x_0$$

2. Simpson's three-eights rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3}{8}h[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

Where $h = \frac{x_3 - x_0}{3}$; $x_1 = x_0 + h$; $x_2 = x_0 + 2h$;

3. Simpson's quadrature formula

$$\int_{x_0}^{x_4} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)]$$

Where $h = \frac{x_4 - x_0}{4}$

4. For N+1 points, where (N/3) is an integer,

$$\int_{x_0}^{x_N} f(x)dx = \frac{3}{8}h[f(x_0) + 3f(x_1) + 3f(x_2) + 2f(x_3) + 3f(x_4) + 3f(x_5) + \cdots + 3f(x_{N-1}) + f(x_N)]$$

Where $h = \frac{x_N - x_0}{N}$

5. For N+1 points, where N is even,

$$\int_{x_0}^{x_N} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 4f(x_{N-1}) + f(x_N)]$$

Where $h = \frac{x_N - x_0}{N}$

Ideal gas constant

$$R = \frac{8.314\ \text{kPa}\cdot.\text{dm}^3}{\text{mol.K}} \qquad R = \frac{1.987\ \text{Btu}}{\text{Ib mol}\cdot^{\circ}\text{R}}$$

$$R = \frac{0.73\ \text{ft}^3\cdot.\text{atm}}{\text{Ib mol}\cdot^{\circ}\text{R}} \qquad R = \frac{8.3144\ \text{J}}{\text{mol.K}}$$

$$R = \frac{0.082\ \text{dm}^3\cdot.\text{atm}}{\text{mol.K}} = \frac{0.082\ \text{m}^3\cdot.\text{atm}}{\text{kmol.K}} \qquad R = \frac{1.987\text{cal}}{\text{mol}\cdot\text{K}}$$

First Point

$$\left.\frac{dC_A}{dt}\right|_{t_0} = \frac{-3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t}$$

Interior Points

$$\left.\frac{dC_A}{dt}\right|_{t_i} = \frac{C_{A(i+1)} - C_{A(i-1)}}{2\Delta t}$$

Last point

$$\left.\frac{dC_A}{dt}\right|_{t_n} = \frac{C_{A(n-2)} - 4C_{A(n-1)} + 3C_{A(n)}}{2\Delta t}$$

Energy balance:

$$T = T_0 + \frac{X\left[-\Delta H_{Rx}(T_0)\right]}{\Sigma\phi_i\tilde{C}_{Pi} + X\Delta\tilde{C}_P}$$

Rate law:

$$k(T) = k(T_1)e^{\left[\frac{E}{R}\left(\frac{1}{T_1}-\frac{1}{T}\right)\right]}$$

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Useful Integrals in Reactor Design

$$\int_0^x \frac{dx}{1-x} = ln\frac{1}{1-x} \qquad (A-1)$$

$$\int_0^x \frac{dx}{(1-x)^2} = \frac{x}{1-x} \qquad (A-2)$$

$$\int_0^x \frac{dx}{1+\varepsilon x} = \frac{1}{\varepsilon} ln(1+\varepsilon x) \qquad (A-3)$$

$$\int_0^x \frac{1+\varepsilon x}{1-x} dx = (1+\varepsilon) ln\frac{1}{1-x} - \varepsilon x \qquad (A-4)$$

$$\int_0^x \frac{1+\varepsilon x}{(1-x)^2} dx = \frac{(1-\varepsilon)x}{1-x} - \varepsilon ln\frac{1}{1-x} \qquad (A-5)$$

$$\int_0^x \frac{(1+\varepsilon x)^2}{(1-x)^2} dx = 2\varepsilon(1+\varepsilon) ln(1-x) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 x}{1-x} \qquad (A-6)$$

$$\int_0^x \frac{dx}{(1-x)(\Theta_B - x)} = \frac{1}{\Theta_B - 1} ln\frac{\Theta_B - x}{\Theta_B(1-x)} \quad \Theta B \neq 1 \qquad (A-7)$$

$$\int_0^x \frac{dx}{ax^2+bx+c} = \frac{-2}{2ax+b} + \frac{2}{b} \quad for\ b^2 = 4ac \qquad (A-8)$$

$$\int_0^x \frac{dx}{ax^2+bx+c} = \frac{1}{a(p-q)} ln\left(\frac{q}{p}\cdot\frac{x-p}{x-q}\right) \quad for\ b^2 > 4ac \qquad (A-9)$$

$$\int_0^W (1-\alpha W)^{1/2}\, dW = \frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right] \qquad (A-10)$$

$$\int_0^\infty \left(e^{-kt}\right)\delta(t-\tau)\, dt = e^{-k\tau} \qquad (A-11)$$

Simpson's five-point formula

$$\int_{x_0}^{x_4} f(x)\, dx = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4\right) \qquad h = \frac{X_4 - X_0}{4}$$